Progress in Large-Scale Differential Variational Inequalities for Heterogeneous Materials

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CMSNF
Center for Materials Science of Nuclear Fuel

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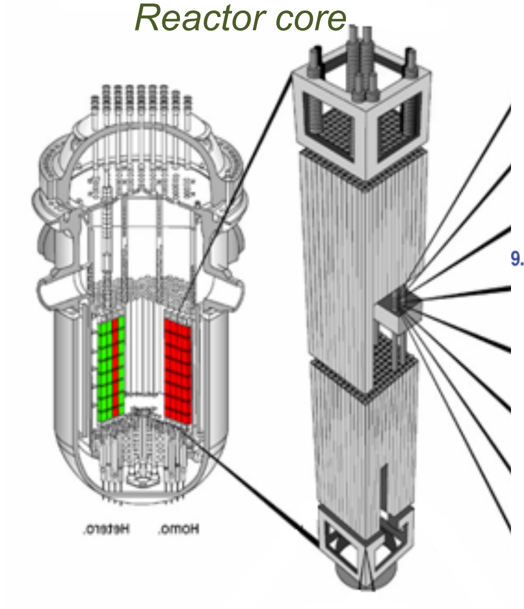
1.Motivation: Study of Materials under Irradiation (A. El Azab)

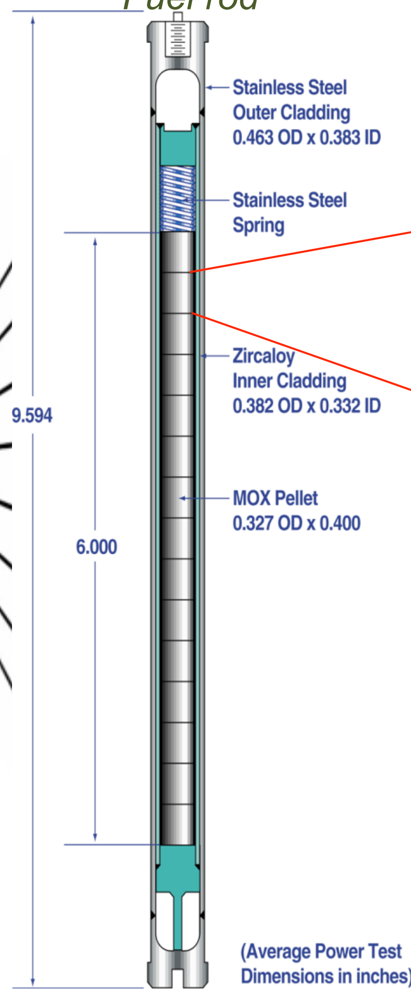
Continuum in irradiated materials

Reactor core



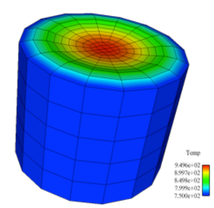
Courtesy C. Degueldre, PSI

Fuel rod

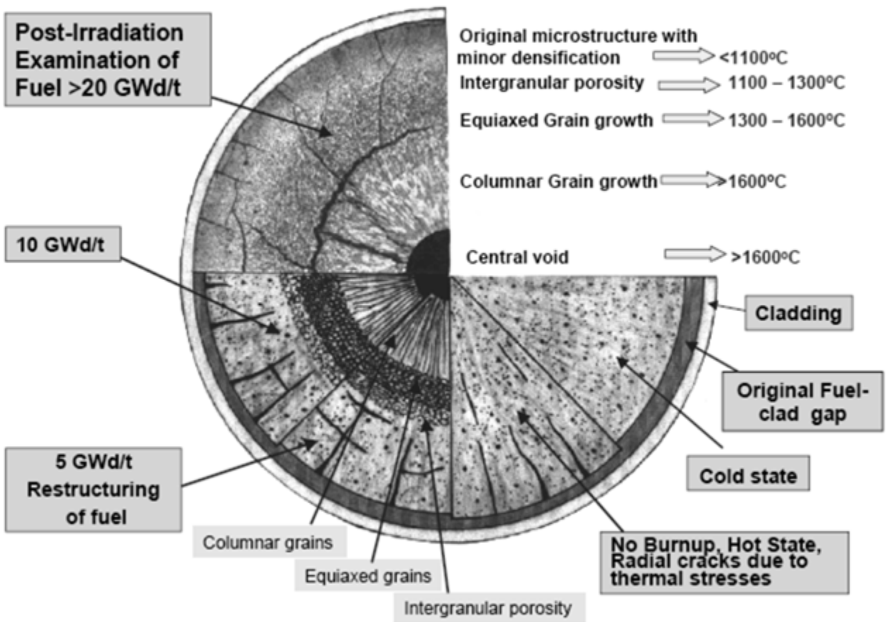


Courtesy J. Carmack, INL

UO_2 fuel pellet

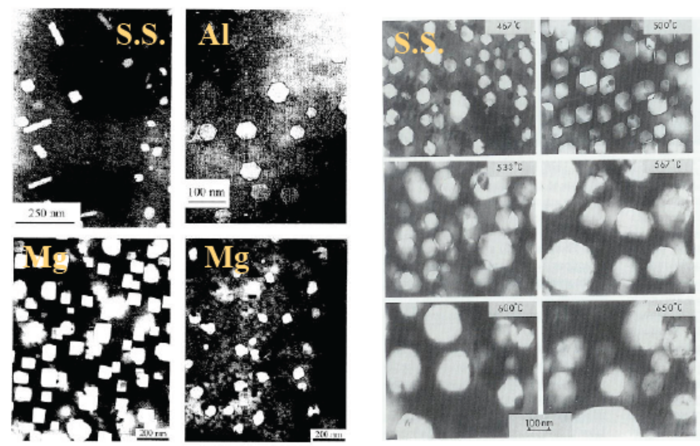


Mesoscale in irradiated materials



Fuel pellet

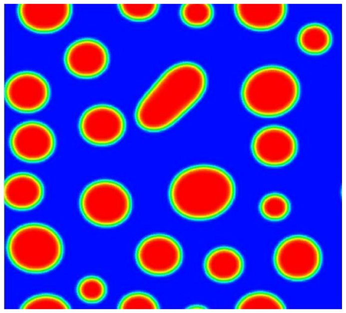
Structural materials



Typical phase field model

From a free energy functional, we derive kinetic equations for composition and microstructure following Onsager formalism of non-equilibrium T.D.

$$\mathcal{E}(c,\eta) = \int_V f(c,\eta)\,d\Omega$$



$$\frac{\partial c}{\partial t} = \nabla \cdot \left(b \nabla \frac{\delta \mathcal{E}}{\delta c} \right) + \xi(x,t)$$

$$\frac{\partial \eta}{\partial t} = -L \frac{\delta \mathcal{E}}{\delta \eta} + \zeta(x,t)$$

Cahn-Hilliard Eq.

Allen-Cahn (G.L.) Eq.

Phase field model for irradiated materials

Appropriate sources and defect reactions are added to represent the irradiation environment and defect process:

modified Cahn-Hilliard Eq.

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(b \nabla \frac{\delta \mathcal{E}}{\delta c} \right) + \xi(x,t) + G(x,t) - R(x,t)$$

modified Allen-Cahn (G.L.) Eq.

$$\frac{\partial \eta}{\partial t} = -L \frac{\delta \mathcal{E}}{\delta \eta} + \zeta(x,t) + \zeta_{\mathrm{Irrad}}(x,t)$$

… if one can compute the functional derivative.

2. The phase field energy. Double well versus double obstacle.

Diffuse boundary model

- We intend to track the evolution of a boundary between phases.
- At the scale of interest the scale of the boundary IS NOT 0, so practically it may not make sense to use a sharp boundary, since its velocity would be very hard to obtain from measurement or theoretical considerations.
- We thus use a phase variable η to define a domain:

$$\mathcal{D} = \{x|\eta(x) = 1\}\ ;\ \mathcal{D}^c = \{x|\eta(x) = 0\}\ ;\ \mathcal{D}^b = \{x|\eta(x) \in (0,1)\}$$

- So the boundary area (between void and matrix, or between grains) is DIFFUSE, such as is the case in real apps.
- Q: How do we model the free energy to accommodate this behavior?

Free energy functional essentials

- Its general form:

$$\mathcal{E} = \int \left[f(c_1, c_2, ..., c_p, \eta_1, \eta_2, ..., \eta_p) + \sum_{i=1}^{n} \alpha_i \left(\nabla c_i\right)^2 + \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{p} \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k \right] d^3 r +$$

$$\int\int G(r_1 - r_2) d^3 r_1 d^3 r_2$$

- How do we deal with the boundary constraints by including an interdiction term on the potential:

$$f(\eta) = f_0 + I(\eta); \;\; I(\eta) = \begin{cases} \infty, & \eta > 1 \text{ or } \eta < 0, \\ 0, & 0 \leq \eta \leq 1 \end{cases}$$

f_0 : smooth, non-convex function

What is the way the interdiction is handled?

- One can replace the potential by a regularized version, called "the double obstacle potential"

$$f(\eta) = 4\Delta f \left(-\frac{1}{2}\eta^2 + \frac{1}{4}\eta^4 \right)$$

- But this introduces stiffness and maybe some non-physical artifacts. If explicit, the time steps can get small, as we have observed for years in contact problems.

- One can do clamping. The way it perturbs the physics is unclear.

- Our solution? Deal with the actual interdiction potential.

- Consequences? Obtain a differential variational inequality.

Cahn-Hillard equations

$f = \Psi$

$$\frac{\partial u}{\partial t} = \nabla \cdot (b(u)\nabla(-\gamma\Delta u + \Psi'(u))) \quad \text{in} \quad \Omega_T := \Omega \times (0, T)$$
$$u(x,0) = u_0(x) \quad \forall x \in \Omega$$
$$\frac{\partial u}{\partial \nu} = b(u)\frac{\partial}{\partial \nu}(-\gamma\Delta u + \Psi'(u)) = 0 \quad \text{on} \quad \partial\Omega \times (0, T)$$

$\rightarrow$

$$\frac{\partial u}{\partial t} = \nabla \cdot (b(u)\nabla\omega) \quad \text{in} \quad \Omega_T$$
$$-\gamma\Delta u + \Psi'(u) = \omega$$

An implicit free boundary where potential becomes infinite, not quite specified. But DVI - WEAK is:

$$\left(\frac{\partial u(x,t)}{\partial t}, \chi_1\right) = (\nabla \cdot (b\nabla w), \chi_1) \quad \forall \chi_1 \in S$$

VI

$$(-\gamma\Delta u + \Psi'(u), \chi_2 - u(x,t)) \geq (w, \chi_2 - u(x,t)) \quad \forall \chi_2 \in K$$

Properly defined everywhere by choosing S,K

Systems of Allen-Cahn equations

$$\boldsymbol{u}_t = b(\boldsymbol{u})\left(\gamma\Delta\boldsymbol{u} - P\nabla_{\boldsymbol{u}}\Psi(\boldsymbol{u})\right)$$

$$P: \quad P\boldsymbol{v} = \boldsymbol{v} - \frac{1}{N}(\boldsymbol{v}\cdot 1)1 \qquad G = \{\boldsymbol{v} \in \mathbb{R}^d | v_i \geq 0, \sum_{i=1}^{N} v_i = 1\}$$

$$b(u) = 1 \qquad \Psi(\boldsymbol{u}) = \begin{cases} \sum_{i<j} u_i u_j, & \boldsymbol{u} \in G, \\ \infty, & \text{otherwise.} \end{cases}$$

Obstacle potential

Weak form tracks diffuse boundary between the two phases $u = 0$ and $u = 1$ where PDE is not defined.

$$(\boldsymbol{u}_t, \boldsymbol{v}) + \gamma(\nabla\boldsymbol{u}, \nabla(\boldsymbol{v} - \boldsymbol{u})) - (\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{u}) \geq -\frac{1}{N}(\mathbf{1}, \boldsymbol{v} - \boldsymbol{u}) \quad \forall \boldsymbol{v} \in \mathcal{G}$$

$$\mathcal{G} := \{\boldsymbol{v} \in H^1(\Omega)^N | \boldsymbol{v}(x) \in G \text{ a.e. in } \Omega\}$$

Motivation

- The problem one wants to solve is a differential variational inequality, but for algorithmic difficulty people go with double well potential.
- Can DVI work?
- Challenges
  - Lack of software for large-scale DVIs
  - Prevailing (non-DVI) approach approximates dynamics of phase variable using a smoothed potential: Stiff problem and undesirable physical artifacts
    - phase field variable does not have a compact support
    - boundary between phases is no longer localized
  - Or it does a clamping whose effect is hard to fathom.
- Hypothesis: Creating Scalable DVI solvers will address important physics problems consistently and efficiently.

3. Time-Stepping Schemes

Finite element discretization Cahn-Hilliard (for the weak form)

$$\left(\frac{u^n - u^{n-1}}{\Delta t}, \chi_1\right)^h + \left(b(u^{n-1})\nabla\omega^n, \nabla\chi_1\right) = 0 \;\; \forall \chi_1 \in S^h$$

$$\gamma(\nabla u^n, \nabla(\chi_2 - u^n)) + (\Psi'(u^n), \chi_2 - u^n) \geq (\omega^n, \chi_2 - u^n)^h \;\; \forall \chi_2 \in K^h$$

$$S^h := \{\chi \in C(\bar{\Omega}) : \chi|_\kappa \text{ is linear } \forall \kappa \in \tau^h\} \subset H^1(\Omega)$$

$$K^h := \left\{\chi \in S^h : 0 \leq \chi \leq 1 \text{ in } \Omega\right\}$$

Complementarity formulation Cahn-Hilliard

$$0 = M_0 \frac{\boldsymbol{u}^n - \boldsymbol{u}^{n-1}}{\Delta t} + M_1 \boldsymbol{\omega}^n$$
$$0 = \gamma M_2 \boldsymbol{u}^n + \psi_1'(\boldsymbol{u}^n) M_0 - \theta_c M_0 \boldsymbol{u}^n + \psi_2'(\boldsymbol{u}^{n-1}) M_0 - M_0 \boldsymbol{\omega}^n + \boldsymbol{\lambda} - \boldsymbol{\mu}$$
$$0 \le \boldsymbol{\lambda} \perp 1 - \boldsymbol{u}^n \ge 0$$
$$0 \le \boldsymbol{\mu} \perp \boldsymbol{u}^n \ge 0$$

$$M_{0\{i,i\}} = (\phi_i, 1)_{L^2(\Omega)}$$
$$M_1(\boldsymbol{u}^{n-1})_{\{i,j\}} = \left(b(u^{n-1}(x_i))\nabla\phi_i, \nabla\phi_j\right)_{L^2(\Omega)}$$
$$M_{2\{i,j\}} = (\nabla\phi_i, \nabla\phi_j)_{L^2(\Omega)}$$

FE/complementarity formulation of Allen-Cahn

For each component $\boldsymbol{u}_i$

$$(\boldsymbol{u}_i^n, \boldsymbol{v} - \boldsymbol{u}_i^n)^h + \Delta t \gamma (\nabla \boldsymbol{u}_i^n, \nabla(\boldsymbol{v} - \boldsymbol{u}_i^n)) \geq ((1+\Delta t)\boldsymbol{u}_i^{n-1} - \frac{\Delta t}{N}\mathbf{1}, \boldsymbol{v} - \boldsymbol{u}_i^n)^h$$

$$\boldsymbol{u}_i > 0 \qquad\qquad \sum_{i=1}^{N} \boldsymbol{u}_i = 1$$

$$M_0 \boldsymbol{u}_i^n + \Delta t \epsilon^2 M_2 \boldsymbol{u}_i^n - \left((1+\Delta t) M_0 \boldsymbol{u}_i^{n-1} - \frac{\Delta t}{N} M_0 \mathbf{1}\right) - \boldsymbol{\lambda} - \boldsymbol{\mu} = 0$$

$$0 \leq \boldsymbol{\lambda} \perp \boldsymbol{u}_i^n \geq 0$$

$$\boldsymbol{\mu} \perp \boldsymbol{e}^T \boldsymbol{u}_i^n = 1$$

The time-stepping scheme is formulated in terms of mixed linear complementarity problems

- The mixed linear complementarity problem:

$$\boxed{\begin{aligned} M_{11}x_1 + M_{12}x_2 &= 0 \\ M_{21}x_1 + M_{22}x_2 &= s_2 \\ s_2 \geq 0 \perp x_2 &\geq 0 \end{aligned}}$$

- TAO includes complementarity solvers for mixed linear complementarity problems.

4. Solvers/Environment

Algebraic solvers

- Differential Variational Inequality

Finite element discretization

- Algebraic Variational Inequality (Complementarity Problems)

Newton's method with active set constraint or semi-smooth solver

- Nontrivial Linear Algebraic System

Nested Krylov solvers and preconditioners

- Simple Algebraic Systems

Cahn-Hillard equations

$$\frac{\partial u}{\partial t} = \nabla \cdot (b(u)\nabla(-\gamma\Delta u + \Psi'(u))) \qquad 0 \le u \le 1$$

Algebraic variational inequailty

$$\begin{pmatrix} \delta t \Delta_b^{n-1} & I \\ -I & -\gamma\Delta \end{pmatrix} \begin{pmatrix} w^n \\ u^n \end{pmatrix} = \begin{pmatrix} -u^{n-1} \\ \psi_2'(u^{n-1}) - \theta_c u^{n-1} \end{pmatrix}$$

Block linear systems obtained from TAO active set

$$\begin{pmatrix} \delta t \Delta_b^{n-1} & \tilde{I} \\ -\tilde{I}^T & -\gamma\tilde{\Delta} \end{pmatrix} \begin{pmatrix} w^n \\ \tilde{u}^n \end{pmatrix} = \begin{pmatrix} \dots \\ \dots \end{pmatrix}$$

Simpler algebraic systems via Schur complements

$$\left(\delta t \Delta_b^{n-1} - \frac{\tilde{I}^T \tilde{\Delta}^{-1} \tilde{I}}{\gamma}\right) w^n = \dots$$

Allen-Cahn equations

$$\mathbf{u}_t = \gamma \Delta \mathbf{u} - P \nabla_{\mathbf{u}} \Psi(\mathbf{u}) \qquad u_i \geq 0, \ \sum_i u_i = 1$$

Algebraic variational inequailty

$$\begin{pmatrix} \delta t I & I & & & \\ -I & -\gamma\Delta & & & I \\ & & \delta t I & I & \\ & & -I & -\gamma\Delta & I \\ & -I & & -I & \end{pmatrix} \begin{pmatrix} w_1^n \\ u_1^n \\ w_2^n \\ u_2^n \\ \mu \end{pmatrix} = \begin{pmatrix} \cdots \\ .. \\ .. \\ .. \\ .. \end{pmatrix}$$

Block linear systems from the TAO complementarity active set problems

$$\begin{pmatrix} \delta t I & \tilde{I} & & & \\ -\tilde{I}^T & -\gamma\tilde{\Delta} & & & \tilde{I} \\ & & \delta t I & \tilde{I} & \\ & & -\tilde{I}^T & -\gamma\tilde{\Delta} & \tilde{I} \\ & -\tilde{I}^T & & -\tilde{I}^T & \end{pmatrix} \begin{pmatrix} w_1^n \\ \tilde{u}_1^n \\ w_2^n \\ \tilde{u}_2^n \\ \mu \end{pmatrix} = \begin{pmatrix} \cdots \\ .. \\ .. \\ .. \\ .. \end{pmatrix}$$

Simpler algebraic systems via Schur complements

$$S = \begin{pmatrix} 0 & \tilde{I}_1 \end{pmatrix} \begin{pmatrix} -\delta t I & \tilde{I}_1 \\ \tilde{I}_1^T & -\gamma\tilde{\Delta}_1 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ -\tilde{I}_1^T \end{pmatrix} + \begin{pmatrix} 0 & \tilde{I}_2 \end{pmatrix} \begin{pmatrix} -\delta t I & \tilde{I}_2 \\ \tilde{I}_2^T & -\gamma\tilde{\Delta}_2 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ -\tilde{I}_2^T \end{pmatrix}$$

Schur complement based preconditioners

are often a powerful technique because using right preconditioned GMRES on

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

with preconditioner

$$\begin{pmatrix} A & B \\ 0 & S = D - CA^{-1}B \end{pmatrix}^{-1}$$

converges in at most two iterations with an exact Schur complement solver, Ipsen, SISC, 2001. A nested solver approximately applies S^{-1} by approximately solving

$$\hat{S} = D - C_{\text{approx}}(A)^{-1}B$$

with preconditioned GMRES. Similarly A^{-1} is approximately solved via GMRES.

Coupled Cahn-Hillard and Allen-Cahn example

Block structure of Jacobian for active set or semi-smooth method. Multiple nesting of Schur complement preconditioners can be used to precondition the system efficiently.

$$
\begin{pmatrix}
\delta t \Delta_b^{n-1} & \tilde{I} & & & & & \\
-\tilde{I}^T & -\gamma_{ch}\tilde{\Delta} & .. & .. & .. & .. & \\
 & .. & \delta t I & \tilde{I} & & & \\
 & .. & -\tilde{I}^T & -\gamma_{ac}\tilde{\Delta} & & & \tilde{I} \\
 & .. & & & \delta t I & \tilde{I} & \\
 & .. & & & -\tilde{I}^T & -\gamma_{ac}\tilde{\Delta} & \tilde{I} \\
 & & & -\tilde{I}^T & & -\tilde{I}^T &
\end{pmatrix}
\begin{pmatrix}
w_{ch}^n \\
\tilde{u}_{ch}^n \\
w_{ac^1}^n \\
\tilde{u}_{ac^1}^n \\
w_{ac^2}^n \\
\tilde{u}_{ac^2}^n \\
\mu
\end{pmatrix}
$$

Solvers for complementarity problems

- PATH
  - Extremely robust (sequential) library with a MATLAB interface
  - Solves a linear variational inequality at each iteration to find direction
  - Globalized with a line search using the Fischer-Burmeister merit function
  - Applies sophisticated preprocessing to improve formulation
  - Successfully used to solve general models with up to 100,000 variables
- Semismooth
  - Robust (parallel) solver in TAO and PETSc
  - Reformulates variational inequality as a nonsmooth system of equations
  - Applied Newton's method to the nonlinear system using subdifferential
  - Reduced linear system with a positive diagonal perturbation
  - Globalized with a line search using the Fischer-Burmeister merit function
  - Successfully used to solve PDE-based models with millions of variables
- Active-set
  - Scalable solver in TAO and PETSc
  - Constructs and solves a reduced linear system
  - Linear algebra requirements similar to those for solving the PDE
  - Globalized with a line search using the Fischer-Burmeister merit function
  - For certain symmetric systems, method is equivalent to:
    - Projected gradient step to obtain active set
    - Newton acceleration step for fast convergence
  - Successfully used to solve PDE-based models with millions of variables

Software developments

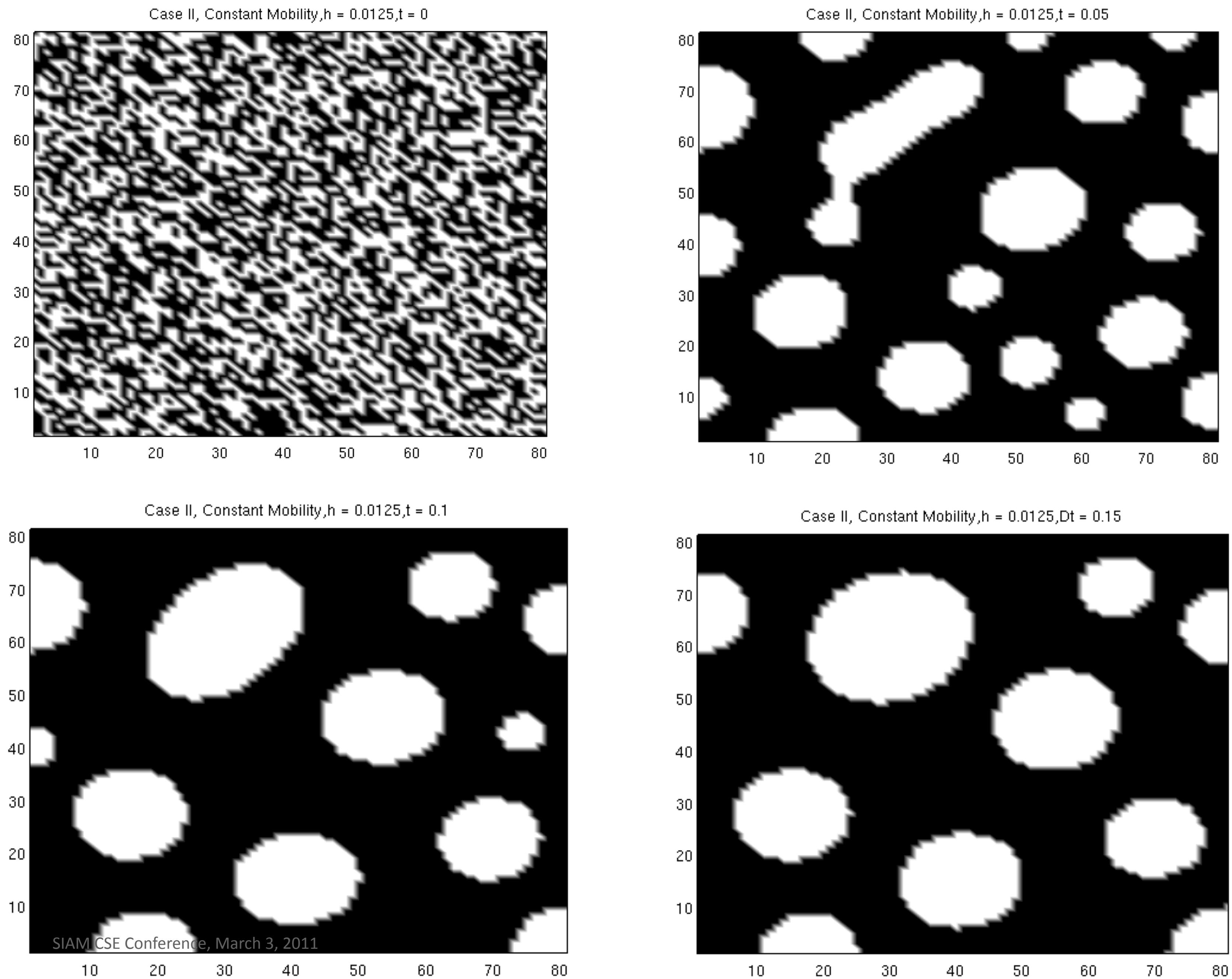
- Solvers (in PETSc):
  - Added SNESVISetVariableBounds(SNES,Vec,Vec)
  - Added two new SNES Newton-based line search subclasses
    - SNESVI active set and SNESVI semi-smooth both use PETSc's flexible linear solver classes, allowing easy use of nested Schur complement solvers.
    - Work requirements of both solvers is O(number of nonzeros in Jacobian) so overall efficiency of and scalability of solvers is determined by efficiency of linear solvers only.
    - Available to entire research community.
- MATLAB interface (sequential):
  - Many applied mathematicians who are not comfortable in FORTRAN or C are experienced with MATLAB.
  - Allows the vectors, Jacobians and nonlinear function evaluations as well as user main program to be provided in MATLAB
  - Scripting language for high user efficiency, rapid prototyping
  - Trivial to use MATLAB's powerful graphics interactively with PETSc

Status

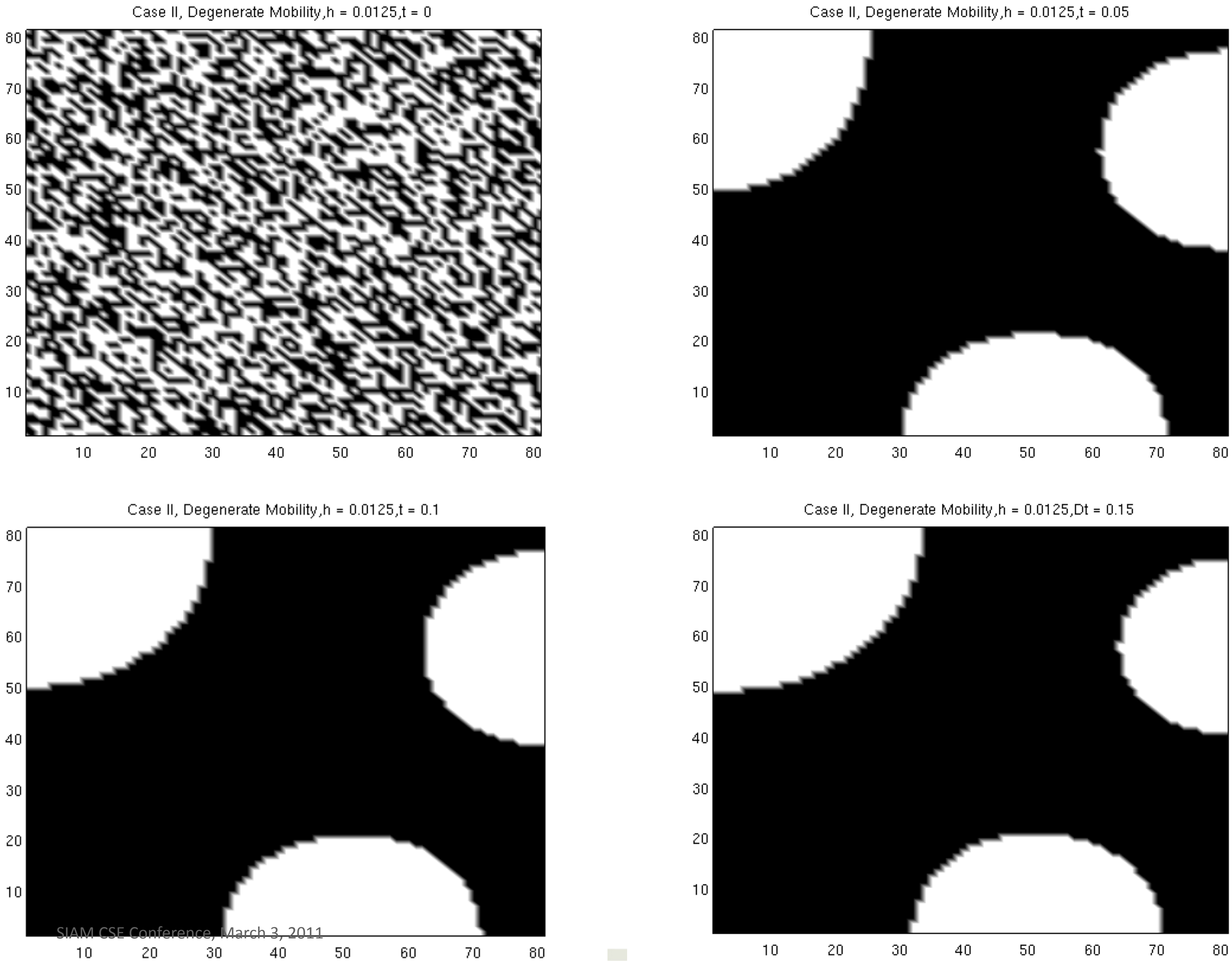
- We can solve 1 and 2 dimensional phase field problems with constant and degenerate mobility as DVI using PETSc.

- Parallel framework comes “for free”

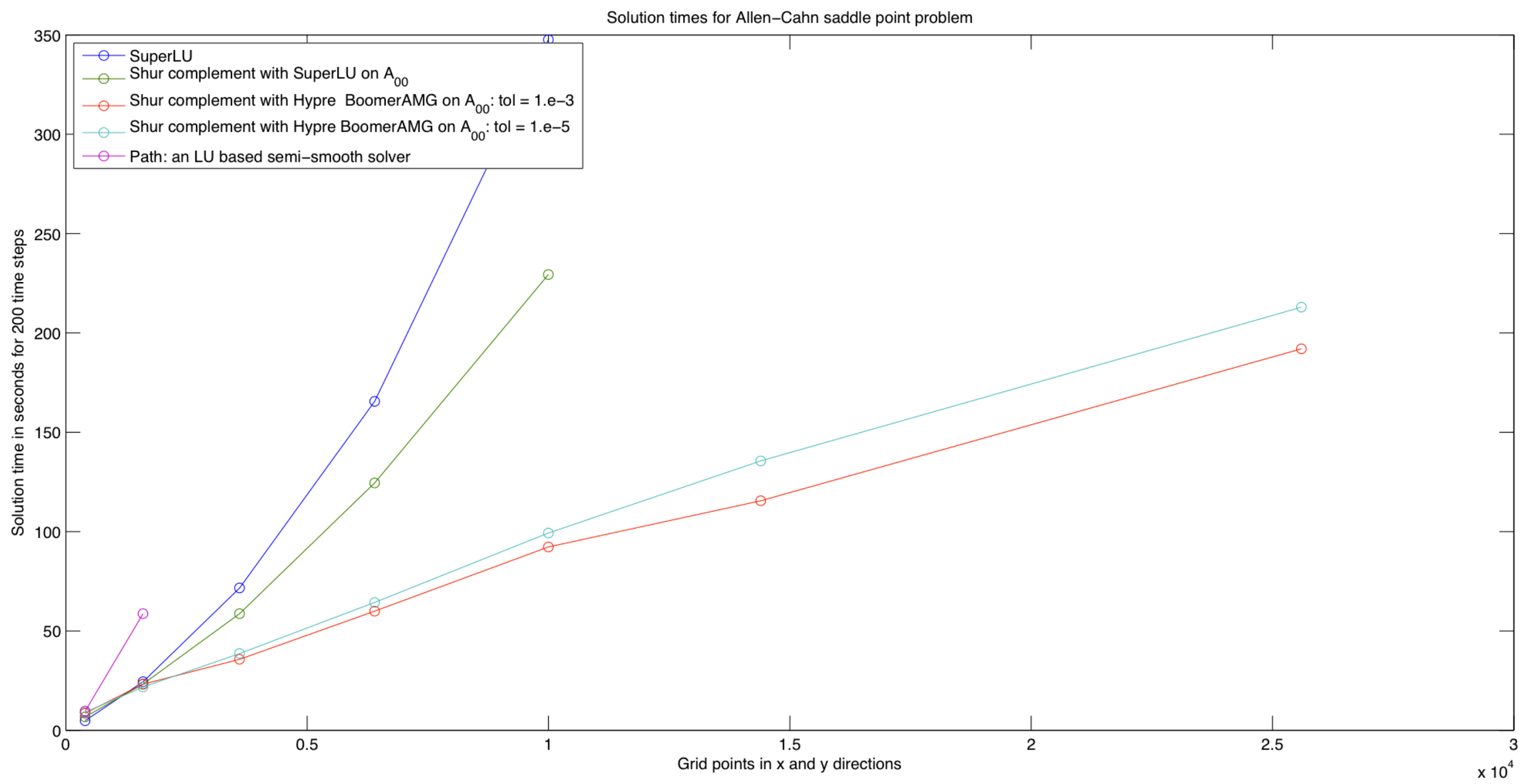
Cahn-Hillard Case III



Cahn-Hillard Case III



Initial scalability tests



5. Numerical Results for Void Formation / Radiation Damage

$$\mathcal{E} = N \int_V \left[h(\eta) f^s(c_v, c_i) + j(\eta) f^v(c_v, c_i) + \frac{\kappa_v}{2} |\nabla c_v|^2 + \frac{\kappa_i}{2} |\nabla c_i|^2 + \frac{\kappa_\eta}{2} |\nabla \eta|^2 \right] dV$$

free energy functional

$$f^s(c_v, c_i) = E_v^f c_v + E_i^f c_i + k_B T [c_v \ln(c_v) + c_i \ln(c_i) + (1 - c_v - c_i) \ln(1 - c_v - c_i)]$$

$$f^v(c_v, c_i) = A \left[(c_v - 1)^2 + c_i^2 \right]$$

$$h(\eta) = (\eta - 1)^2 + \eta^2$$

P. Millett, A. El-Azab, S. Rokkam, M. Tonks, D. Wolf
Comp. Mate. Sci. (50) 2011

$$\frac{\partial c_v}{\partial t} = \nabla \cdot \left(M_v \nabla \frac{\delta \mathcal{E}}{\delta c_v} \right) - R_{iv}(x,t)$$

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(M_i \nabla \frac{\delta \mathcal{E}}{\delta c_i} \right) - R_{iv}(x,t)$$

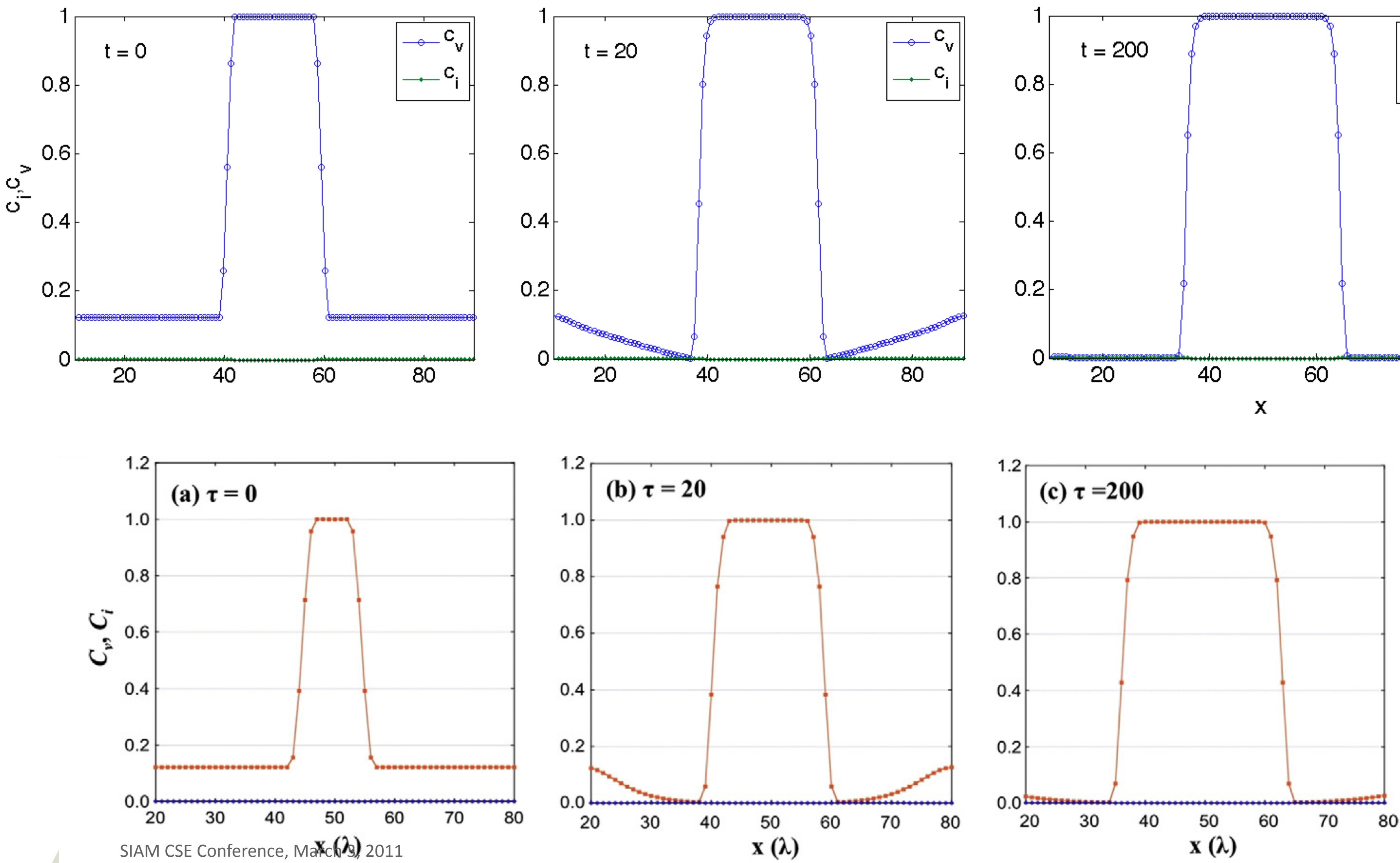
$$\frac{\partial \eta}{\partial t} = -L \frac{\delta \mathcal{E}}{\delta \eta}$$

$$M_v = \frac{D_v c_v}{k_B T} \qquad M_i = \frac{D_i c_i}{k_B T}$$

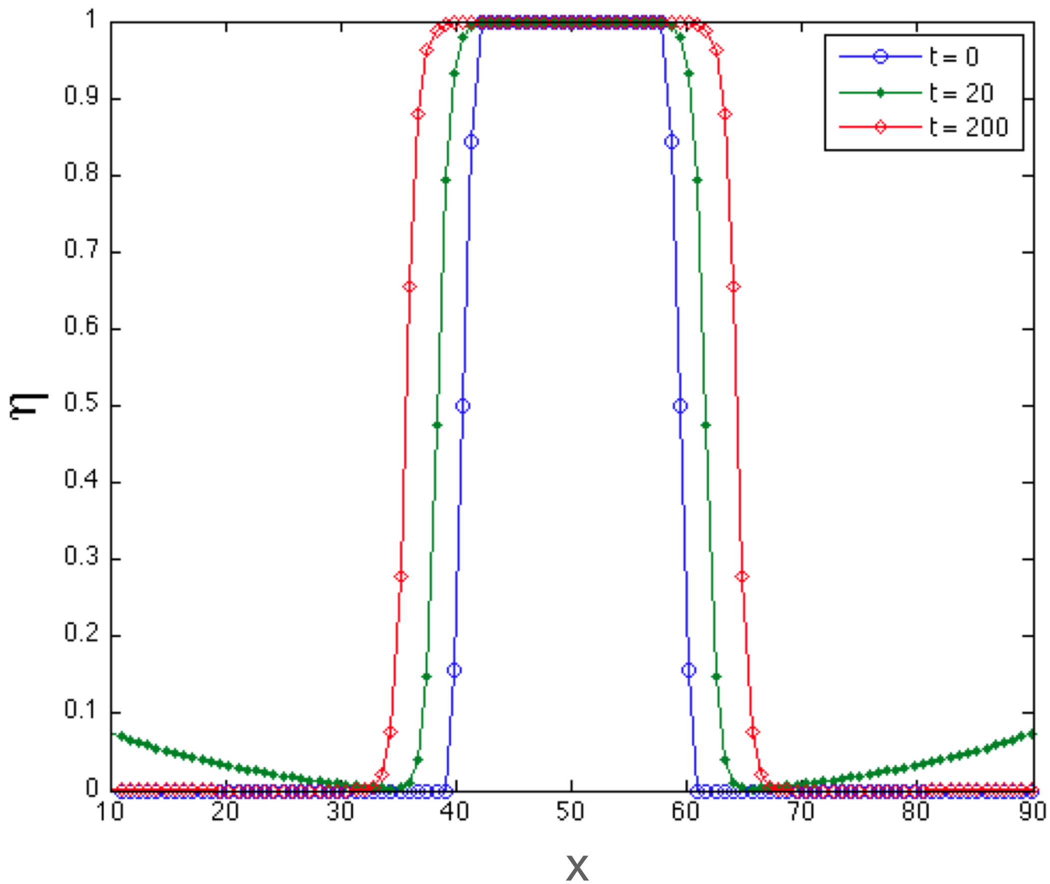
: Degenerate Mobility

$$R_{iv}(x,t) = R_r c_v c_i \qquad R_r = R^{bulk} + \eta^2 \cdot R^{surf}$$

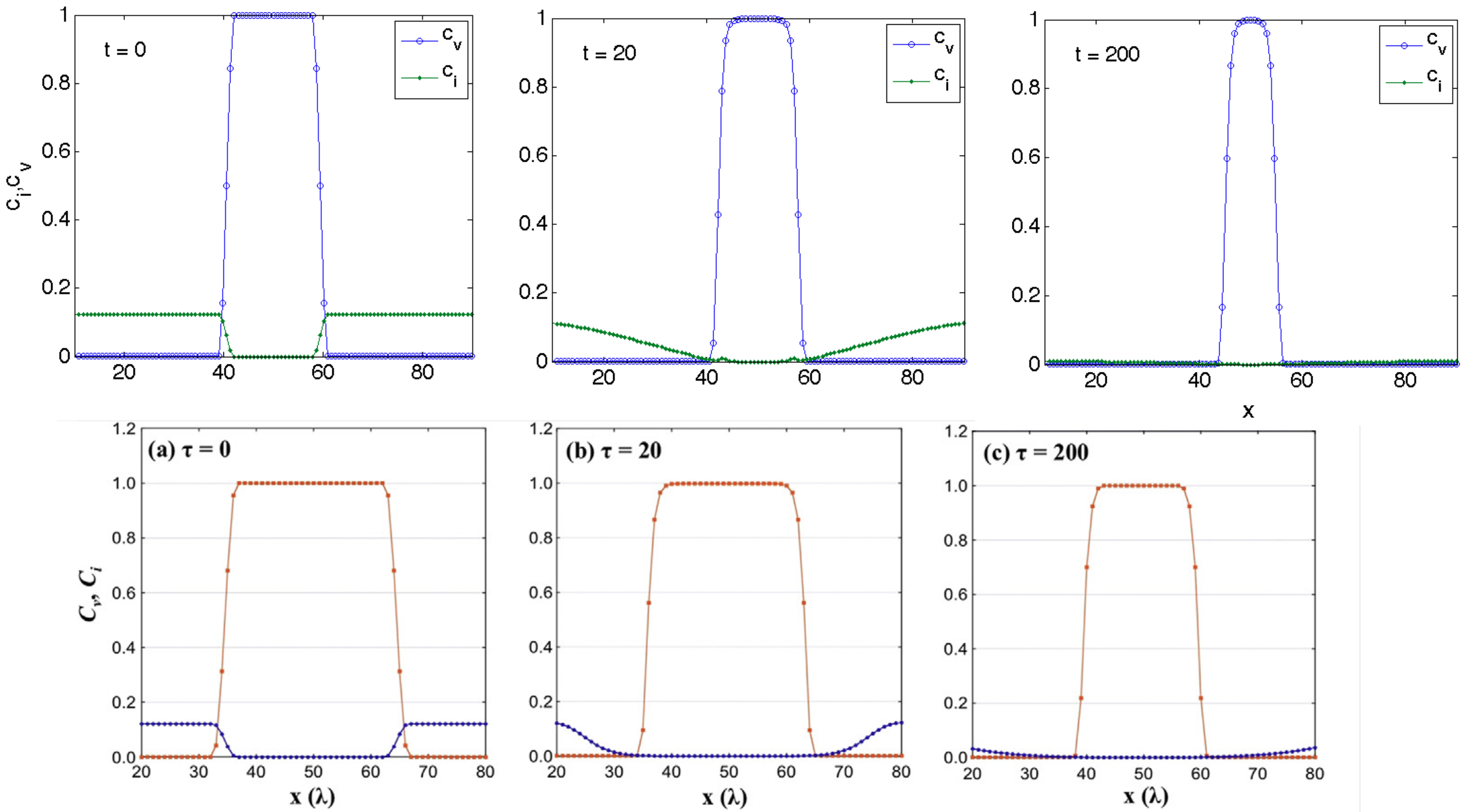
Void Grow : DVI , PATH, Dt = 1e-3



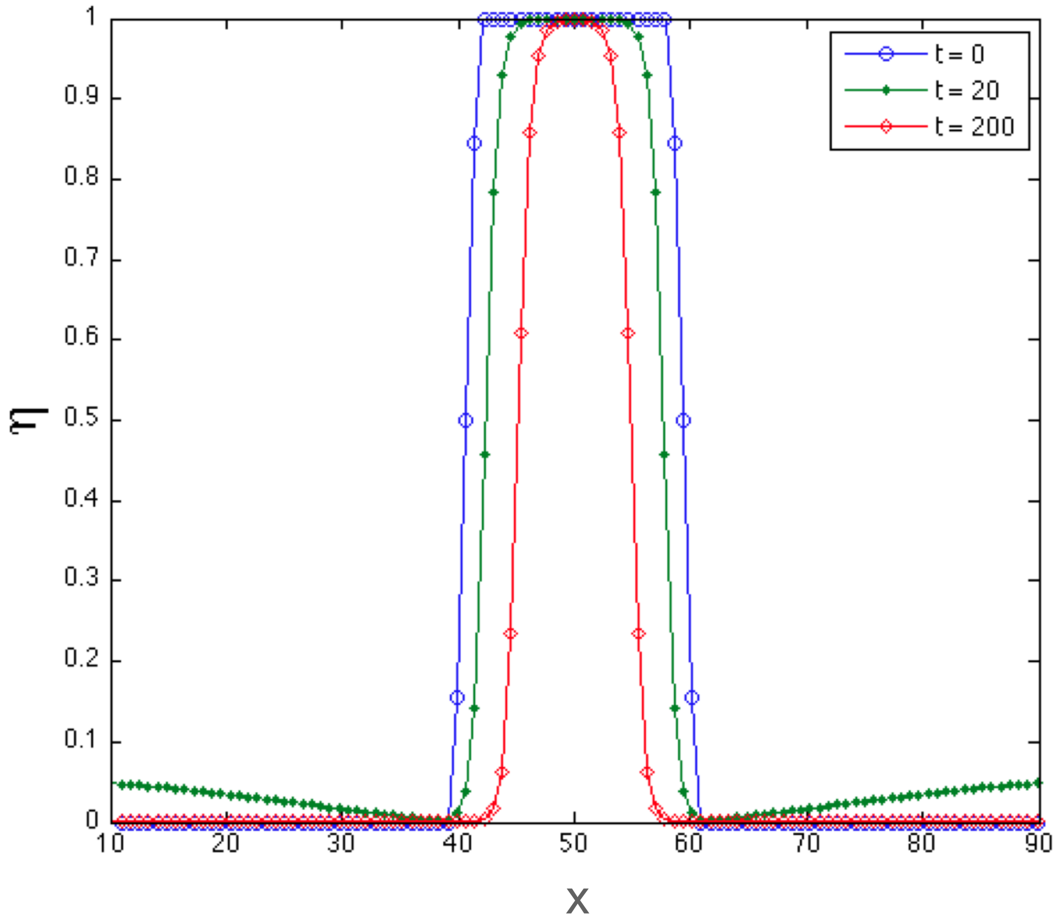
Void Grow : DVI , PATH, Dt = 1e-3



Void Shrink : DVI , PATH, Dt = 1e-3



Void Shrink : DVI , PATH, Dt = 1e-3



Case II

$$\frac{\partial c_v}{\partial t} = \nabla \cdot M_v \nabla \left(-\kappa_v \nabla^2 c_v + \Psi_v'(c_v, \eta)\right)$$

Constant Mobility

$$\frac{\partial \eta}{\partial t} = -L \left(-2\kappa_\eta \nabla^2 \eta + \Psi_\eta'(c_v, \eta)\right)$$

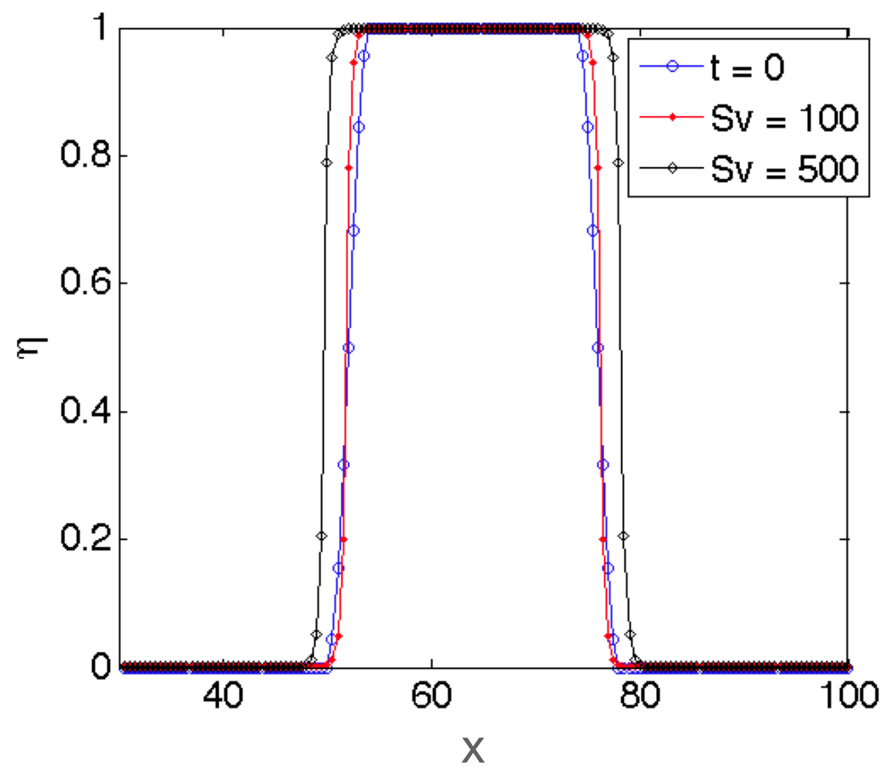
$$\Psi_v'(c_v, \eta) = h(\eta)(E_v^f + \ln c_v - \ln(1 - c_v))$$
$$-2A(c_v - c_v^o)\eta(\eta + 2)(\eta - 1)^2 + 2B(c_v - 1)\eta^2$$

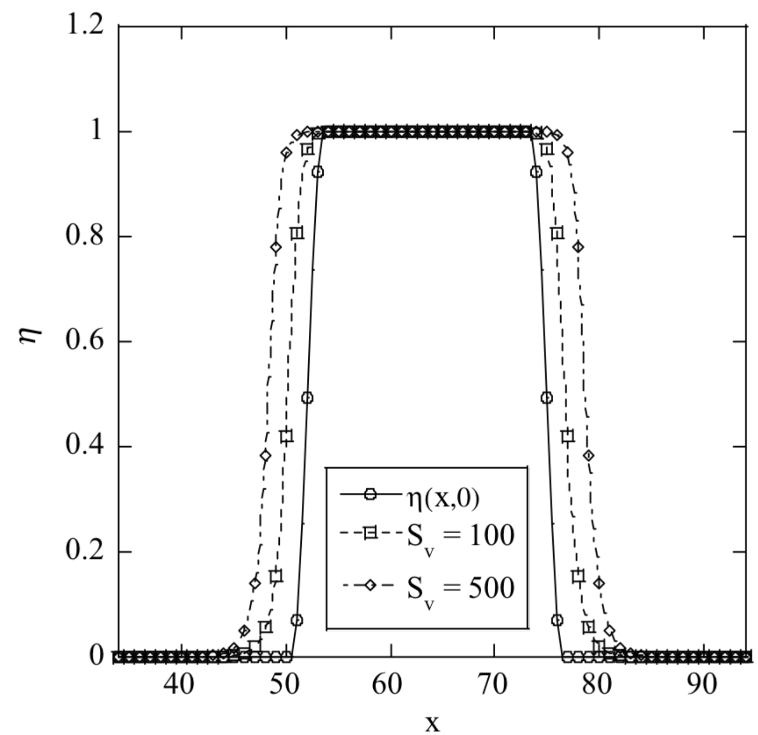
$$\Psi_\eta'(c_v, \eta) = h'(\eta) \left(E_v^f c_v + c_v \ln c_v + (1 - c_v) \ln(1 - c_v)\right)$$
$$-A(c_v - c_v^o)^2(4\eta^3 - 6\eta + 2) + 2B(c_v - 1)^2\eta$$

S.Rokkam, A.Ei-Azab, P.Millett and D.Wolf

Modeling Simul.Mater. Sci.Eng. 17(2009)

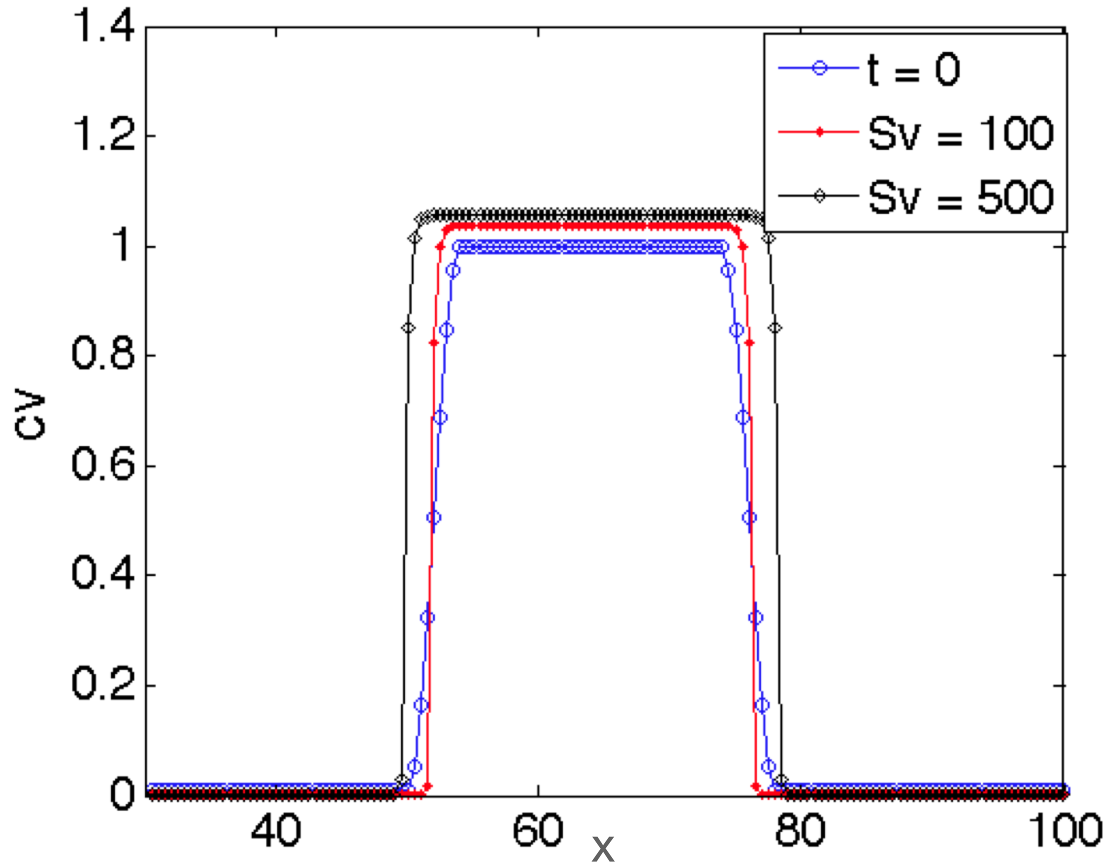
Direct finite difference results





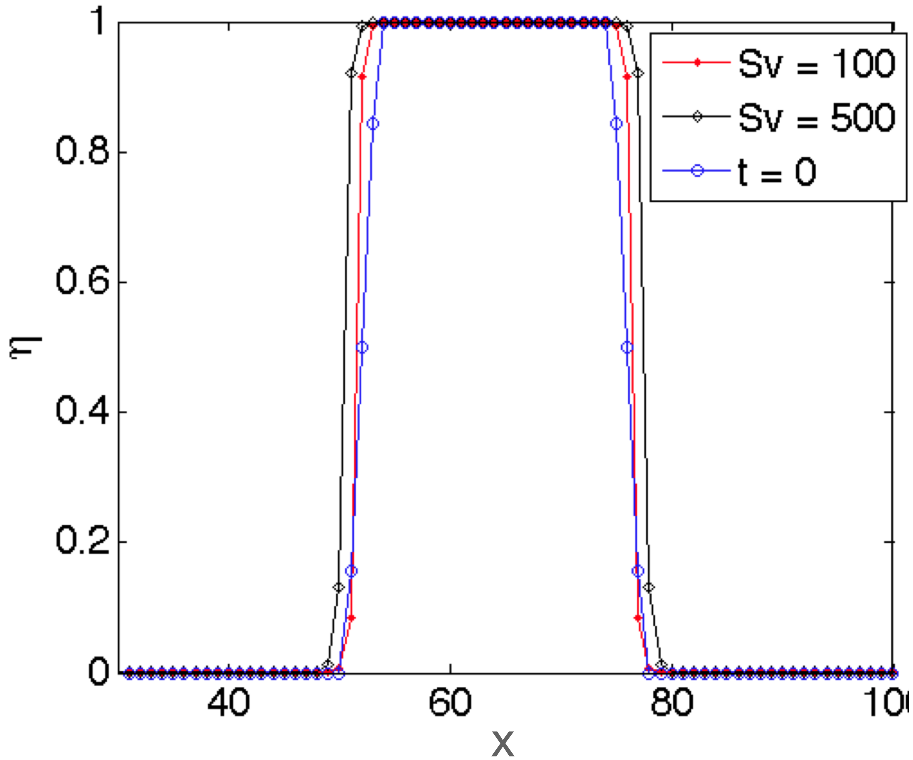
t = 50

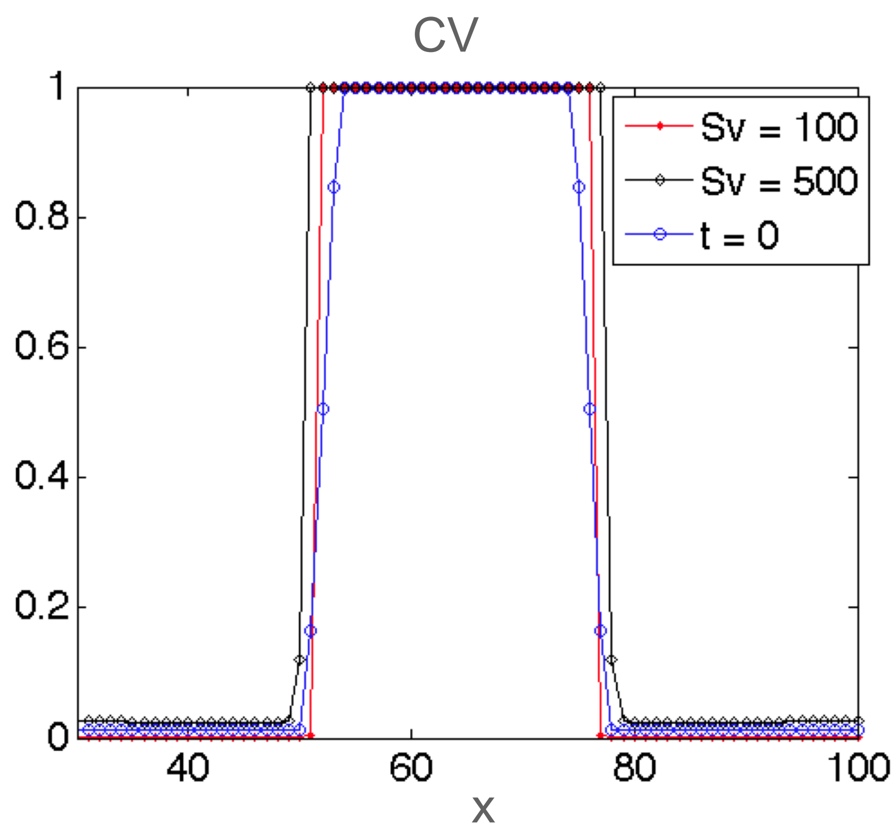
Direct finite difference results



t = 50

DVI + PATH results





Why DVI?

$$G_v(c_v) = E_v^f c_v + k_B T \left[c_v \ln(c_v) + (1 - c_v) \ln(1 - c_v) \right]$$

temperature. (To avoid numerical instabilities, if $c_{\mathrm{v}} \leqslant 0$ the first term in brackets is dropped and a negative sign is assigned to the first term on the rhs. Likewise, if $c_{\mathrm{v}} \geqslant 1$ the second term in brackets is dropped.) The shape function $h(\eta)$ in equation (1) has the expression

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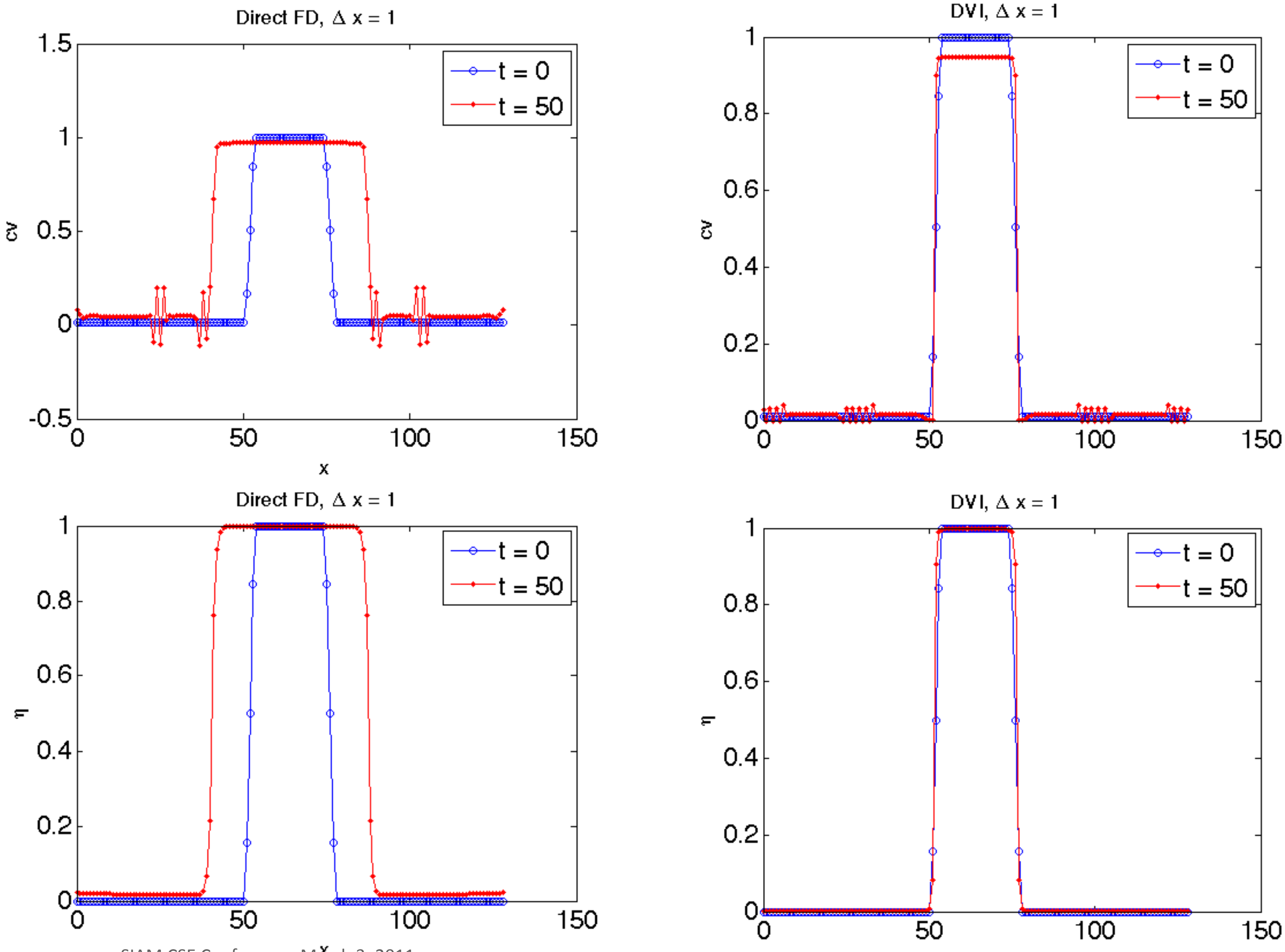
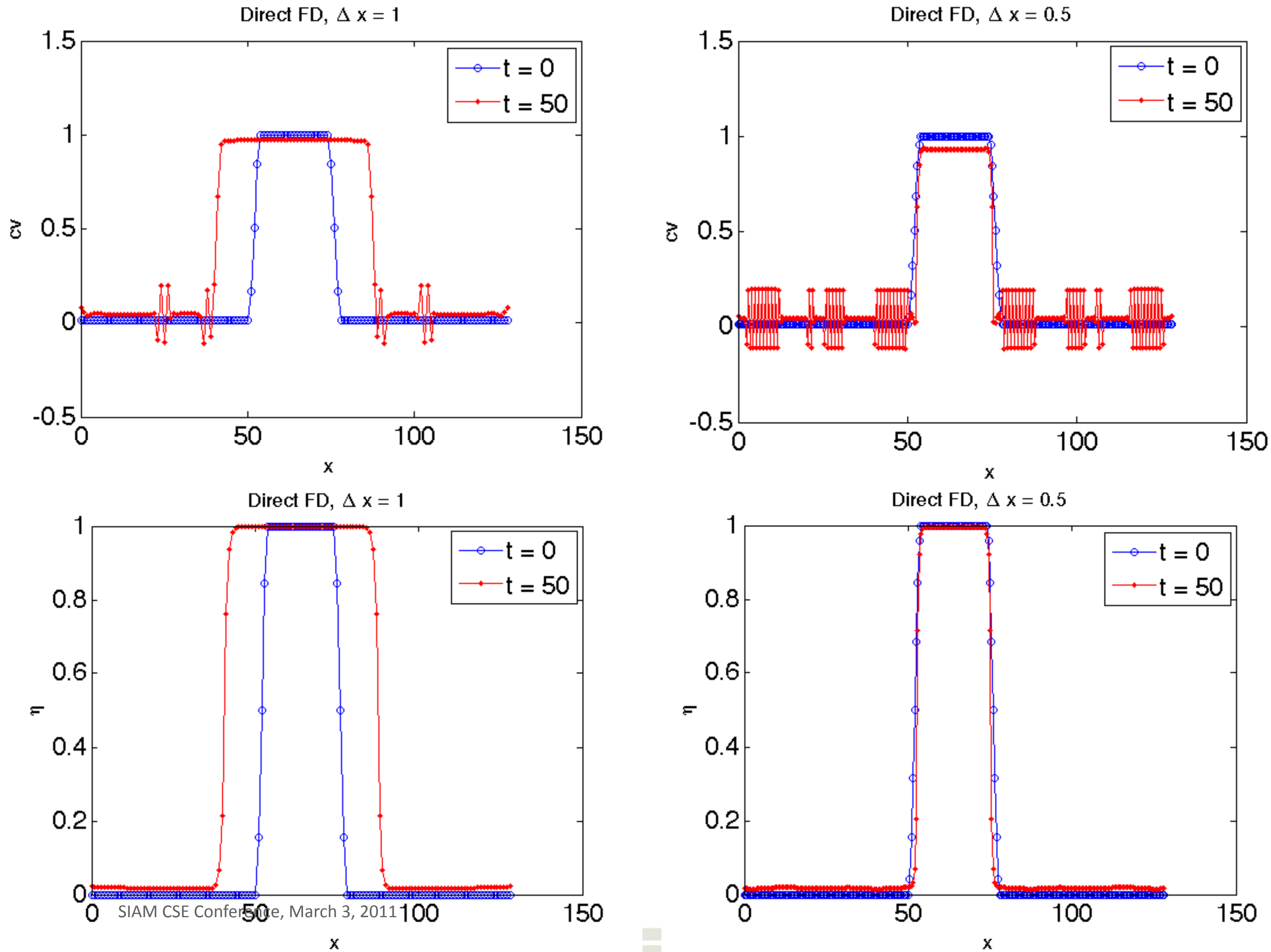
Why DVI?


Direct FD, Δ x = 1
t = 0
t = 50
cv
x
DVI, Δ x = 1
t = 0
t = 50
cv
Direct FD, Δ x = 1
t = 0
t = 50
η
x
DVI, Δ x = 1
t = 0
t = 50
η

Direct FD, Same Dt, Different Dx



Conclusion

- We proposed a DVI formulation and the associated time-stepping schemes.
- We have created initial computational infrastructure for DVI.
- We have proposed a Schur-complement based preconditioning approach. For Allen-Cahn with constant mobility (likely the complexity driver) excellent scalability.
- We have validated it for void formation/radiation damage.
- We have demonstrated it is more stable than clamping.

- Future:
  - Multi-grain parallel, large-scale experiments.
  - Numerical analysis of the DVI approach.
  - Solving large radiation damage problems.
  - Higher-order schemes.
  - Extending to other free boundary physics …
  - We have only scratched the surface on the modeling significance of DVIs.

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